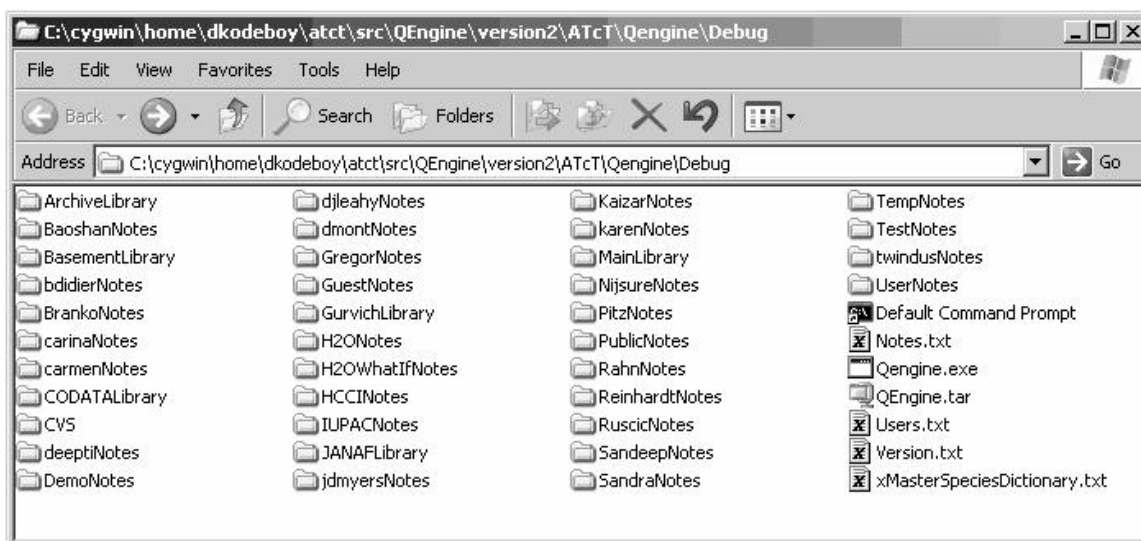


ATcT: Introductory Notes

These notes are to provide the reader with an overview of the inputs, outputs and the functionality of the Active Tables Program. Active Tables is a Fortran program written using the DEC Fortran 90 Windows compiler. Work on moving this over to the Intel compiler is in progress. Active Tables' for usage in science has been discussed in numerous papers. This is more of a what-goes-on behind-the-scenes documentation for developers who want to use active tables. Most of the information has been obtained from discussions with Dr. Branko Ruscic. The portlet-webservice architecture has not been outlined over here.

User Management:

Users are managed by storing their usernames and passwords in the file Users.txt which is in the Qengine directory. The user's file information is stored in Notes.txt located in the same place. This file contains details regarding the username, Usernotes folder name and the notesfolder's password. The user's files are stored in the notesFolder that has been assigned to him in Notes.txt. The figure below is a snapshot of the Qengine directory's contents.



This directory as you can see from the snapshot above contains the userNotes folders and also the libraries in Active Tables. The libraries consist of flat files with standard information that has been published some place or experimentally obtained values. We will come back to these a little later.

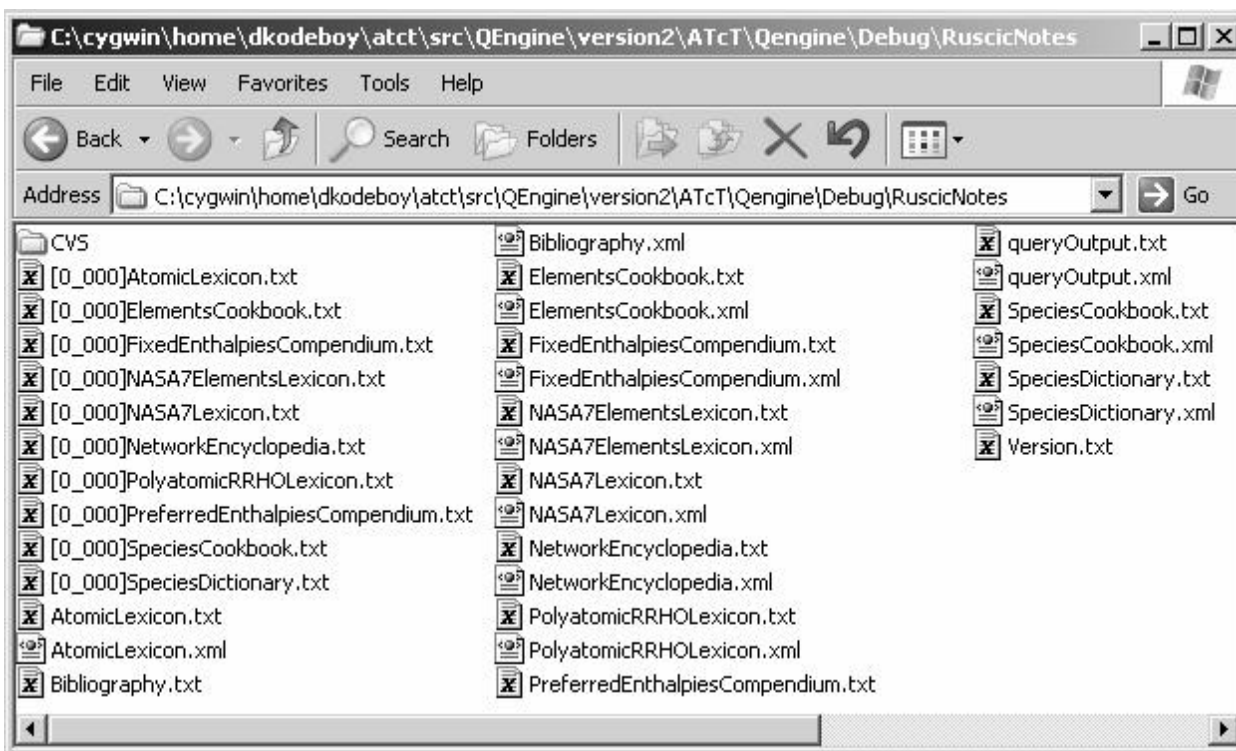
User Notes folder Contents:

Some of the common files in the user notes folder are listed below.

- Elements Cookbook

- Species Dictionary
- Species Cookbook
- Network Encyclopedia
- Fixed Enthalpies Compendium
- Preferred enthalpies compendium
- Bibliography
- Lexicon files
 - Atomic Lexicon
 - NASA7ElementsLexicon
 - NASA7Lexicon
 - Polyatomic RRHO Lexicon

Different data is stored in each of these files and the format of each of these files and their purpose will be described below.



Species Dictionary:

The species dictionary contains the species original CAS no., formula and alternative names. In any query to active Tables the species may be referred to by a formula, CAS no or a name that is listed in the species dictionary. For example, a snippet from the species dictionary has been listed below. Here, the CAS no., formula and alternative names have been listed in the same order.

H+
Hydrogen atom cation
Hydrogen cation
Atomic hydrogen ion (1+)
Proton
p+

Species Cookbook:

The species cookbook contains the phase information for all the species listed in the species dictionary. Using the same H+ example from above, the corresponding listing in the species cookbook is:

12408-02-5
H+
12408-02-5*0
H+ <g>
12408-02-5*100
H+ <aq>

The cookbook lists all the phases that the species can exist in and an extension is added to the species CAS no. to provide a unique ID. The extensions are consistently defined for each phase. Negative CAS numbers are assigned for species that are not available in any of the other libraries.

Network Encyclopedia:

The Network encyclopedia is responsible for storing information about the reactions that make up the network. The reactions are all balanced. ATcT gives an error when unbalanced equations are added into the network. Every reaction in this file has some data associated with it besides the reactants and products. This includes the enthalpy of formation or the Gibb's energy, the uncertainty, the temperature and the reference information. The units for all these values are also stored here. A sample reaction is as below:

1 {CH3 <g>, 2229-07-4} + 1 {O2 <g>, 7782-44-7} -> 1 {CH3OO <g>, 2143-58-0}
-96.5 14.4 298.15 kJ/mol DG [884,1003]
-115.3 10.2 298.15 kJ/mol DH [884,1002]
-96.9 8.4 298.15 kJ/mol DG [882]
-137.0 3.8 298.15 kJ/mol DH [881]

Every reaction can have many differing values from different sources as shown in the above example. The reaction itself contains the reactants and products, their phase, their CAS number along with the extensions if applicable.

Fixed Enthalpies Compendium:

This file contains the species whose enthalpies are to be kept fixed when the network is being solved for the enthalpy values for the other unknowns. This can be changed before each solve figure out the extent of change some species may bring upon the entire network. Here again the CAS number, species formula, phase, enthalpy, uncertainty and temperature information is stored.

```
10035-10-6  
HBr <g>  
-36.29 0.16 298.15 kJ/mol [11]
```

Preferred Enthalpies Compendium:

This file contains the unknown species information as a result of the solve function. The format is just the same as the Fixed enthalpies compendium file but these species are the output of solve.

Bibliography:

The literature reference information for the Active tables network is stored here. This information is simply to maintain some pedigree information for data in active tables.

Lexicon Files:

The lexicon files contain more specie specific information like the partition function, vibration frequency etc.

Libraries:

There are also various libraries with species data and their own network information stored in the library folders. These can also be used by the user when searching for species information by adding these to his path using the “set path” command. The hierarchy of this search will determine the order in which the search is executed.

Functionality:

The main function of the Active Tables program is to deliver the thermochemical information for species that are unknown using the current fixed values. Based on the dependencies that exist, the program will solve the network to deliver this to the user. User's enter new reactions and use species information that is already present in other libraries if they do not want to provide any updated information. Any information provided by the user has to be added in the appropriate file in the userNotes folder. After the network has been created successfully the active tables program can solve for the unknowns. The output is stored in the preferred enthalpies file as already described. This is the basic working of the system.